PROGRESS REPORT

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The research effort of Slemrod has been directed to developing a discrete velocity kinetic theory model for liquid-vapor phase transitions. The work engaged approximately 75% of Slemrod's ONR research time. The aim of the research is to develop a "basic principles" description of liquid-vapor phase transitions (such as those occurring in an internal combustion engine) which is not a priori biased by ad hoc equations of state (constitutive relations).

The modelling is almost completely finished, numerical simulations are being run, and a first draft of the results is being written. The model is of the following form:

We consider a gas of clusters in three dimensional space made up monomers, dimers, trimers, etc. which can move with seven fixed momenta: the six unit vectors $\pm i$, $\pm j$, $\pm k$ plus the $\underline{0}$ vector. The clusters can collide elastically and inelastically. The elastic collisions conserve mass, momentum, and energy. The inelastic collisions occur when clusters coagulate or fragment and conserve mass and momentum. In an inelastic collisions kinetic energy is lost. This represents the transfer of kinetic energy to the binding energy of the larger cluster formed in such an inelastic collisions. To keep matter simple the inelastic collisions are of a very simple type, i.e. Becker-Doring cluster kinetics which allow for clusters to gain (lose) only a monomer in coagulations (fragmentations).

A set of transport equations has been written down and analyzed especially as respects propagation of liquid-vapor interfaces. The model was slso solved numerically in collaboration with A. Qi (Univ. of Wisconsin) and M. Grinfeld (Univ. of Bristol, England).

Results were also (favorably) compared with laboratory experiments.

We are now engaged in improving the model to more fully account for the liquid phase. The natural way to do this is to allow the Becker-Doring cluster coefficients to depend in a feedback fashion on the local density. In other words the ability of a gas to coagulate and fragment will be impeded at high densities. This feedback mechanism seems to be a rather straightforward idea though perhaps new to the kinetic theory of gases.

Slemrod reported on his work at the "Workshop on Metastability", Heriot-Watt University, Edinburgh, U.K. July 8, 9, 1993. The workshop was particularly useful to Slemrod since he was able to engage in discussions with Prof. Oliver Penrose, F.R.S., on the implementation of the feedback mechanism.

Slemrod devoted 25% of his time to comparing two viscosity mechanisms in the study of hyperbolic systems of conservation laws. The issue is as follows:

If one wishes to solve the Riemann problem for a hyperbolic system of conservation laws

(1) $u_t + f(u)_x = 0 \quad -\infty < x < \infty,\ t > 0$ with Riemann data

(2) $u(x,0) = \begin{cases} u_- & x < 0 \\ u_+ & x > 0 \end{cases}$

it is natural to expect the solution to depend only on the similarity variable $\xi = \frac{x}{t}$. This is because the change of variables $x \to \alpha x,\ t \to \alpha t,\ \alpha > 0$, leaves (1), (2) unchanged and so the solution should depend only on the ratio of x to t.

On the other hand it is natural to try to solve (1), (2) as a "viscous limit" of the system

(3) $u_t + f(u)_x = \varepsilon u_{xx}$

(4) $u(x,0)=\begin{cases} u_- & x<0 \\ u_+ & x>0 \end{cases}$

as $\varepsilon \to 0_+$. But (3), (4) does not possess the space time dilational invariant of (1), (2), i.e. $x \to \alpha x$, $t \to \alpha t$ does indeed change (3), (4). In order to circumvent this difficulty (C. M. Dafermos [1]) suggested a self-similar viscosity formulation

(5) $u_t + f(u)_x = \varepsilon t u_{xx}$

(6) $u(x,0)=\begin{cases} u_- & x<0 \\ u_+ & x>0 \end{cases}$

which does possess the desired space-time dilational invariance. This allows a search for solutions of (5), (6) of the form $v(\xi)$ so that v satisfies the system of ordinary differential equations

(7) $-sv'(\xi)+f(v)'=\varepsilon v''$, $-\infty<\xi<\infty$,

(8) $v(-\infty)=u_-$, $v(+\infty)=u_+$.

In [1] Dafermos demonstrated applicability of these ideas to systems of two equations. This was followed by work of Dafermos, Dafermos and DiPerna, Fan, Slemrod, Slemrod and Tzavaras. But the question remains what is the meaning of the system (5), (6), i.e. how do solutions of (5), (6) compare with those of the "real system" (3), (4)?

In new research Slemrod has begun answering these questions by viewing the problem as one of stability under perturbation in right sides, i.e. εu_{xx} changed to εt_{xx}. The problem is put in a Hamilton-Jacobi format and estimates are done at that level in a spirit developed for stability of travelling waves given by J. Goodman [2]. So far Slemrod has applied his idea to Burgers' equation

$$u_t + \left(\frac{u^2}{2}\right)_x = \varepsilon u_{xx} \tag{9}$$

where shocks and rarefaction waves are the solutions of the Riemann problem.

The result is roughly that away from $t = 0$ the solution of (7), (8) and solution of (3), (4) differ by an amount proportional to $\sqrt{\varepsilon}\log\varepsilon$, i.e. the two solutions have the same limit as $\varepsilon \to 0_+$.

The importance of this research is it allows us to confidently use analogous self-similar viscosities in other more difficult problems, i.e. spherically symmetric solutions of the three dimensional Euler equations for isentropic, inviscid flow where ξ will be r/t, r the distance from the origin of a spherically symmetric solution.

References

[1] C. M. Dafermos, Solution of the Riemann Problem for a Class of Hyperbolic Conservation Laws by the Viscosity Method, Arch. Rat. Mech. Analysis **52** (1973), 1-9.

[2] J. Goodman, Nonlinear Asymptotic Stability of Viscous Shock Profiles for Conservation Laws, Arch. Rat. Mech. Analysis **95** (1986), 325-344.